propyl 1-naphthylacetate

551-04-2 | DTXSID00286261

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 51.1 °C

Global applicability domain: Inside

Local applicability domain index: 8.61e-01

Confidence level: 5.62e-01

Nearest Neighbors from the Training Set

Image not found
Ethyl 1-naphthaleneacetate
Measured: 88.5
Predicted: 56.1

Image not found
2-Phenylethyl phenylacetate
Measured: 26.5
Predicted: 51.8

Image not found
Ethyl 2-naphthoate
Measured: 32.0
Predicted: 56.0

Image not found
p-Tolyl benzoate
Measured: 71.5
Predicted: 57.4

Image not found
Benzyl benzoate
Measured: 21.0
Predicted: 54.9